Effect of phase breaking on the ac response of mesoscopic systems

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Recently, there have been a number of interesting experiments on the ac response of mesoscopic systems. An important question in this context concerns the characteristic frequency at which the conductance deviates from the dc value. Depending on the system under consideration, this frequency is determined by the following three parameters: the inverse of the average time an electron spends inside the device, the thermal frequency, and the inverse of the phase-breaking time. The theoretical work in this area has been largely based on the scattering formulation, which neglects phase-breaking processes. The purpose of this paper is to derive a more general formulation that allows us to incorporate phase breaking. This formulation is based on the nonequilibrium-Green's-function formalism and we use double-energy coordinates, which helps establish the relation to scattering theory. We illustrate the effect of phase breaking by two simple examples: a one-dimensional resonant-tunneling device with a single resonant level and a resonant-tunneling device with two resonant levels.

I. INTRODUCTION

An important question regarding the ac response of mesoscopic systems is the characteristic frequency ω_c at which the conductance deviates from the dc value. There are three relevant parameters: the inverse of the time an average electron spends inside the device (τ_d^{-1}), the inverse of the phase-breaking time (τ_ϕ^{-1}), and the thermal frequency ($k_B T/\hbar$). How these parameters influence the characteristic frequency is likely to depend on the system under consideration. For example, recent experiments on disordered metallic films[1] have shown that the weak localization correction to conductivity is reduced when $\omega \sim \tau_\phi^{-1}$. On the other hand, experiments on gold rings[2] show that the h/e Aharonov-Bohm oscillations in the conductance persist to frequencies in excess of τ_d^{-1} (which must be much greater than τ_ϕ^{-1} in order for Aharonov-Bohm oscillations to be visible), leading the authors to suggest that it might be the thermal frequency that determines the characteristic frequency.

On the theoretical side, several authors have studied transient transport in mesoscopic systems.[3-15] Reference 9 provides a formulation for the small-signal conductance based on scattering theory. It shows that if we apply a small ac voltage v_{ac} to contact 1 (Fig. 1), then the ac currents i_α, $\alpha \in 1,2$, is given by

$$i_\alpha(\omega) = \frac{e^2}{h} \int dE \, \mathrm{Tr}[I\delta_{\alpha,1} - s_{\alpha 1}^\dagger(E + \hbar\omega)s_{\alpha 1}(E)]$$
$$\times v_{ac} \frac{f(E) - f(E + \hbar\omega)}{\hbar\omega} , \qquad (1)$$

where s is the scattering matrix of the device and f is the equilibrium Fermi function. Here it is assumed that there is no ac potential in the conductor itself. The formulation can be extended to remove this assumption. It is important to note that i_α denotes only the conduction currents at the contacts, which do not sum up to zero.

Their sum is equal to the time rate of change of charge Q stored inside the device:

$$i_1 + i_2 = \frac{dQ}{dt} = I_D . \qquad (2)$$

Depending on how the image charge is distributed among the contacts, the displacement current (I_D) distributes itself among the different leads, providing overall current conservation.

Equation (1) provides a simple approach for investigating the ac linear response of phase-coherent mesoscopic systems. However, this formulation assumes coherent transport and thus cannot be used to investigate the effect of phase-breaking processes on the ac response. To elucidate this point, we consider a one-dimensional resonant tunneling diode [Fig. 2(a)]. The transmission coefficient can be written as $s_{21}(E) = \sqrt{\Gamma_1 \Gamma_2}/[(E - E_r) + i(\Gamma_1 + \Gamma_2)/2]$. From Eq. (1), in the high-temperature limit ($k_B T \gg \hbar\omega$ and $\Gamma_1 + \Gamma_2$) we obtain

$$i_2 = \frac{e^2}{\hbar} \frac{\Gamma_1 \Gamma_2}{\Gamma_1 + \Gamma_2 - i\hbar\omega} f' v_{ac} , \qquad (3)$$

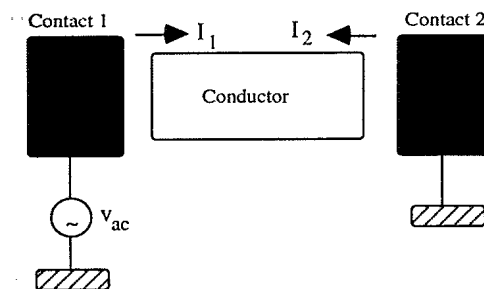which illustrates the well known fact that the characteris-

FIG. 1. Two-terminal mesoscopic conductor with an ac voltage applied to one of the contacts.

tic frequency of a phase-coherent resonant-tunneling diode is determined by $(\Gamma_1+\Gamma_2)/\hbar$, which can be identified with τ_d^{-1}. Here $f' \equiv \partial f /\partial E$ is evaluated at the resonance energy. However, it is straightforward to see
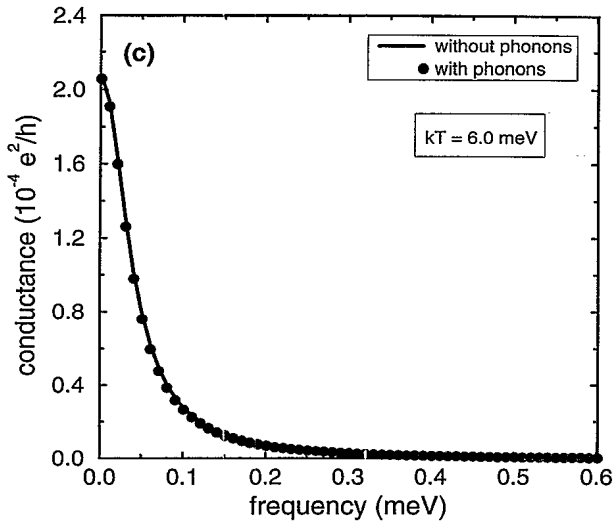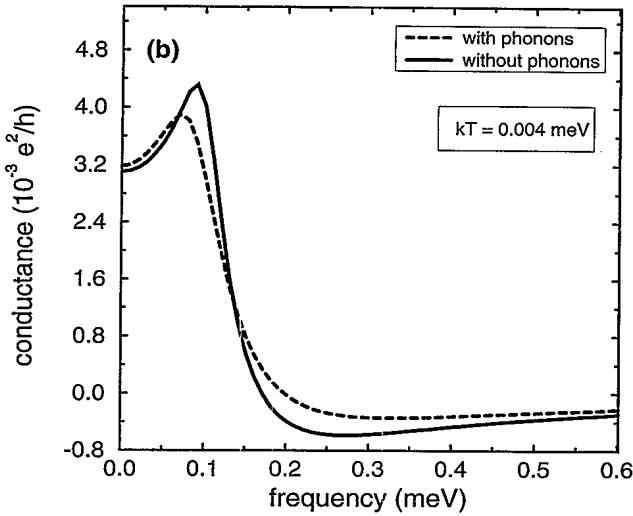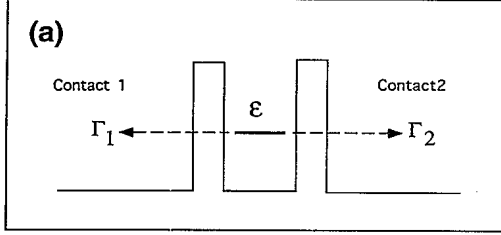
(a)

Contact 1   Contact2

ε

Γ_1 ◄ $\longrightarrow$ Γ_2

(b)   ---- with phonons
               —— without phonons

kT = 0.004 meV

conductance (10^{-3} e^2/h)

frequency (meV)

(c)   —— without phonons
               ● with phonons

kT = 6.0 meV

conductance (10^{-4} e^2/h)

frequency (meV)

FIG. 2. (a) Plot of a one-level resonant-tunneling device. ϵ=5.0 meV, Γ_1=Γ_2=0.02 meV, μ=4.9 meV, and D=0.12 meV. (b) Real part of the linear response conductance (i_2/v_{ac}) as a function of frequency without (solid) and with (dashed) phase-breaking scattering for kT=0.004 meV. (c) The real part of the linear-response conductance (i_2/v_{ac}) as a function of frequency without (solid) and with (solid circles) phase-breaking scattering for kT=6.0 meV.

that we run into difficulty if we attempt to incorporate phase breaking. It is well known that in the presence of phase-breaking processes the transmission coefficient is modified to $s_{21}(E)=\sqrt{\Gamma_1\Gamma_2}/[(E-E_r)+i(\Gamma_1+\Gamma_2+\Gamma_\phi)/2]$, where $\Gamma_\phi=\hbar/\tau_\phi$. A naive application of Eq. (1) would yield

$$i_2=\frac{e^2}{\hbar}\frac{\Gamma_1\Gamma_2}{\Gamma_1+\Gamma_2+\Gamma_\phi-i\hbar\omega}f'v_{ac} \; .$$

If this were correct, the characteristic frequency would increase due to phase-breaking processes from $(\Gamma_1+\Gamma_2)/\hbar$ to $(\Gamma_1+\Gamma_2+\Gamma_\phi)/\hbar$. This is, however, clearly wrong. In the high-temperature regime $(k_BT \gg \hbar\omega$ and $\Gamma_1+\Gamma_2)$ the device can be described using a rate equation based on the sequential model $(f' \equiv \partial f /\partial E)$:

$$i_1=\frac{e}{\hbar}\Gamma_1(f'ev_{ac}-Q), \quad i_2=\frac{e}{\hbar}\Gamma_2 Q, \quad i_1+i_2=\frac{dQ}{dt} \; , \quad (4)$$

which yields exactly the same expression for current as the phase-coherent case [Eq. (3)]. Clearly, then, phase-breaking processes cannot increase the characteristic frequency of a resonant tunneling device as one might expect from a naive application of Eq. (1). In this paper we give a formulation to calculate the ac response of mesoscopic systems including *phase-breaking* scattering. There has been some work[3,6] on including phase-breaking processes that is based on the Kubo formalism, which uses the fluctuation-dissipation theorem to relate the linear-response conductance to the equilibrium noise. The nonequilibrium-Green's-function (NEGF) formalism, on the other hand, deals directly with the transport problem and is applicable even in far-from-equilibrium situations. Recently Refs. 8, 12, and 16 provided a formulation based on the NEGF formalism. Our formulation is similar to Refs. 8, 12, and 16, but we use double-energy coordinates,[17] which makes the connection to scattering theory more transparent. For example, scattering by a time-dependent potential causes an incident electron at energy E to transmit to a different energy E'. In the NEGF formalism, this process is described by a double-energy retarded Green's function $G^r(E,E')$, which plays the role of the transmission coefficient $t(E,E')$. This relationship would be obscured by the use of the double-time Green's function. This physical picture is valid while describing motion of quasiparticles in any ground state and the concept of two energy arguments has been used in Ref. 18 in the context of superconductivity. Moreover, the use of double-energy coordinates allows us to incorporate the proper boundary conditions in a form similar to that used in the scattering formulation. As a result, it is easy to show that our formulation reduces to the scattering formulation when phase-breaking processes are neglected. We illustrate our formulation by applying it to the resonant-tunneling device discussed above [Fig. 2(a)] and to a resonant-tunneling device with two energy levels E_1 and E_2 [Fig. 3(a)], which exhibits two peaks in the conductance $G(\omega)$, one at ω=0 and the other at ω=$(E_2-E_1)/\hbar$ [Fig. 3(b)]. Interestingly, phase breaking has no effect on the first peak, but changes the frequency response of the second peak.
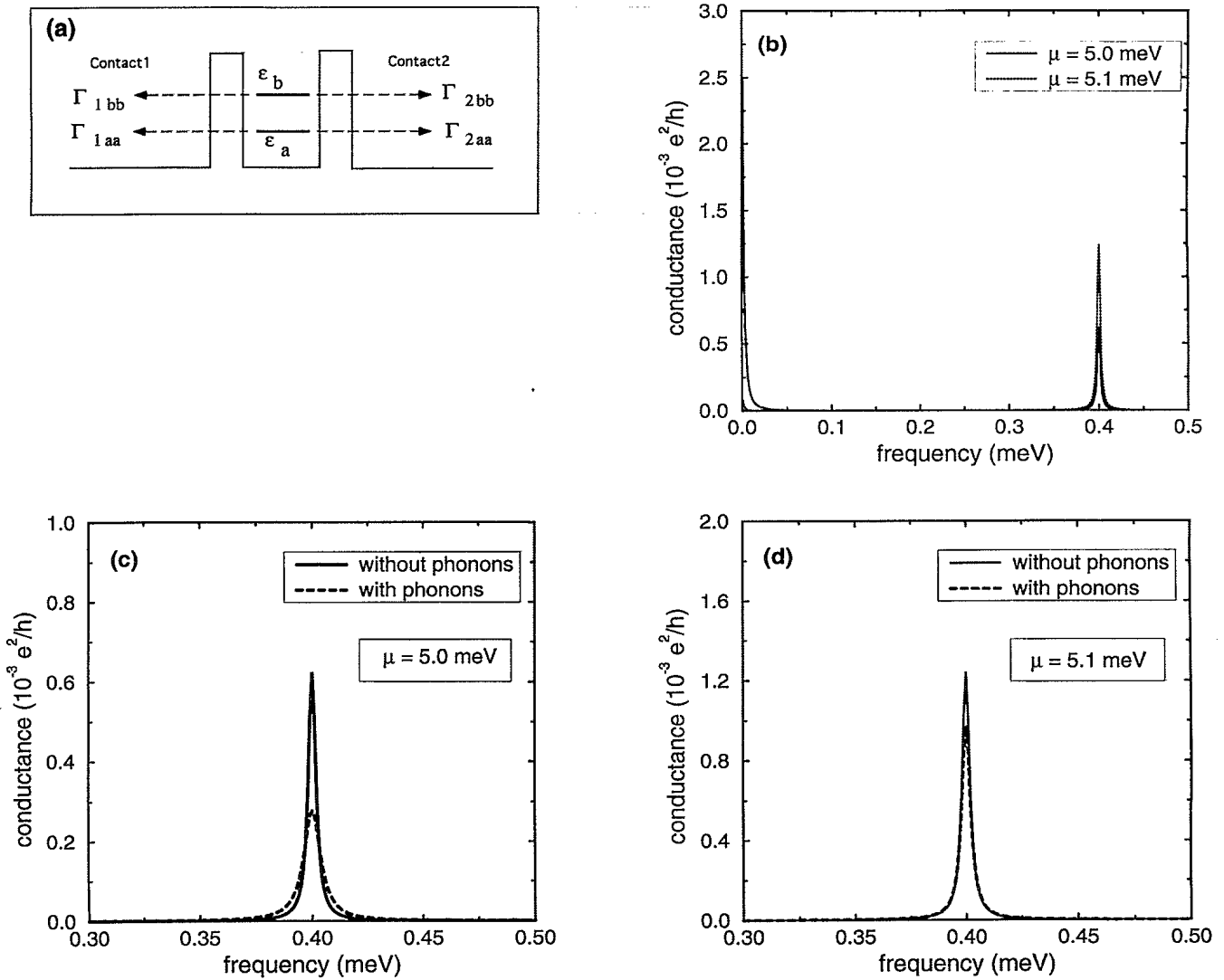
FIG. 3. (a) Plot of a one-dimensional resonant tunneling diode with two resonant levels. The parameters chosen are $\epsilon_a = 5$ meV, $\epsilon_b = 5.4$ meV, $\Gamma_{1aa} = \Gamma_{2aa} = \Gamma_{1bb} = \Gamma_{2bb} = \Gamma_{1ba} = \Gamma_{2ab} = 1 \times 10^{-3}$ meV, $\Gamma_{\phi b} = 5\Gamma_{1aa}$, $kT = 0.04$ meV, and $D = 0.005$ meV. (b) Plot of the conductance (i_2/v_{ac}), in units of e^2/h, versus frequency, assuming no phase-breaking scattering. The solid line is plotted with the chemical potential $\mu = 5.0$ meV $= \epsilon_a$ and the dotted line is plotted with $\mu = 5.1$ meV $> \epsilon_a$. (c) Plot of the high-frequency conductance, in units of e^2/h, versus frequency, with (dashed) and without (solid) phase-breaking scattering. Apart from the reduction in peak height, the width of the frequency response increases due to phase breaking. $\mu = 5$ meV $= \epsilon_a$. (d) Plot of the high-frequency conductance, in units of e^2/h, versus frequency. Here difference in ac conductance with (dashed) and without (solid) phase breaking is small compared to (c). $\mu = 5.1$ meV $> \epsilon_a$.

II. GENERAL FORMULATION

A. Expression for the current

To calculate the conduction current we use the method initiated by Caroli et al.:[19,20,8,12] The system initially consists of an unconnected device region (H_D) and the contacts $(H_{C\alpha})$; the coupling $(V_{C\alpha})$ between the device and contact α is introduced as a perturbation. The Hamiltonian is of the form

$$H(t) = H_D(t) + \sum_{\alpha \in \text{ contacts}} H_{C\alpha}(t) + V_{C\alpha}(t) .$$

Both electron-electron and electron-phonon interactions

in the device can be included in H_D, the Hamiltonian of the device region. The chemical potential and externally applied time-dependent voltages in the contacts are assumed to be known exactly. The fact that the rate of change of electron density $[Q(t) = eN(t)]$ in the device equals the sum of conduction currents through all the contacts can be used to derive an expression for the conduction current:

$$\frac{dQ(t)}{dt} = \frac{e}{i\hbar}[N, H]_- = \sum_\alpha J_\alpha^C, \quad J_\alpha^C = \frac{e}{i\hbar}[N, V_{C\alpha}]_- . \quad (5)$$

Equation (5) is obtained by noting that the commutator bracket $[N, H]_- = \sum_\alpha [N, V_{C\alpha}]_-$. This is because the

terms H_C and H_D cannot change the number of electrons in the device. To evaluate the right-hand side of Eq. (5) we work in the tight-binding representation and assume the following forms for $V_{C\alpha}$ and $H_{C\alpha}$:

$$H_{C\alpha} = \sum_i \epsilon_{i\alpha,i\alpha}(t)\psi_{i\alpha}^\dagger(t)\psi_{i\alpha}(t)$$
$$+ \sum_{i\neq j} t_{i\alpha,j\alpha}(t)\psi_{i\alpha}^\dagger(t)\psi_{j\alpha}(t) + \text{c.c.} , \quad (6)$$

$$V_{C\alpha} = \sum_i V_{i\alpha,x}(t)\psi_{i\alpha}^\dagger(t)d_x + \text{c.c.}$$

Here $\psi_{i\alpha}(t)$ [$\psi_{i\alpha}^\dagger(t)$] refer to electron creation [annihilation] operators including spin at site i of contact α. $d_x^\dagger(t)$ [$d_x(t)$] are creation [annihilation] operators including spin at site x of the uncoupled device region. Applying a sinusoidal potential $v_{ac}\cos(\omega t)$ to contact α causes the site energies in contact α to vary as $\epsilon_{i\alpha}(t) = \epsilon_{i\alpha} + v_{ac}\cos(\omega t)$. The matrix element connecting the contact to the device, $V_{i\alpha,x}(t)$, is now time dependent. Making use of the fact $N(t) = \sum_{x\in \text{device}} d_x^\dagger(t)d_x(t)$, we have, from Eq. (5),

$$J_\alpha(t) = \sum_{i,x} V_{i\alpha,x}(t)G_{x,i\alpha}^<(t,t) - V_{i\alpha,x}^*(t)G_{i\alpha,x}^<(t,t) , \quad (7)$$

where $G_{x,i\alpha}^<(t,t) = i\langle \psi_{i\alpha}^\dagger(t)d_x(t)\rangle$, $G_{i\alpha,x}^<(t,t) = i\langle d_x^\dagger(t)\psi_{i\alpha}(t)\rangle$, and $G_{x,i\alpha}^>(t,t) = -i\langle \psi_{i\alpha}(t)d_x^\dagger(t)\rangle$ are the usual Green's functions appearing in the NEGF formulation.[21,22] The Green's function appearing on the right-hand side of Eq. (7) connects the device and the contacts. However, the real value of this method initiated by Caroli et al. lies in the fact that the current can be expressed in terms of the unperturbed Green's function in the contacts and the full Green's functions only in the device region. The following important relations derived in Refs. 8 and 20 help express the current in this form:

$$G_{x,i\alpha}^<(t,t) = \sum_{x'\in \text{device}} \int_{-\infty}^{+\infty} dt_1 V_{x',i\alpha}^*(t_1)$$
$$\times [G_{x,x'}^r(t,t_1)G_{i\alpha,i\alpha}^{0<}(t_1,t)$$
$$+ G_{x,x'}^<(t,t_1)G_{i\alpha,i\alpha}^{0a}(t_1,t)] , \quad (8)$$

$$G_{i\alpha,x}^<(t,t) = \sum_{x'\in \text{device}} \int_{-\infty}^{+\infty} dt_1 V_{i\alpha,x'}(t_1)$$
$$\times [G_{i\alpha,i\alpha}^{0r}(t,t_1)G_{x',x}^<(t_1,t)$$
$$+ G_{i\alpha,i\alpha}^{0<}(t,t_1)G_{x',x}^a(t_1,t)] ,$$

where $G_{i\alpha,i\alpha}^{0k}(t,t_1)$, $k\in r$, and $a, >, <$ are the unperturbed Green's functions[23] in contact α. Using Eqs. (8) and the relationship $G^r(t_1,t_2) - G^a(t_1,t_2) = G^>(t_1,t_2) - G^<(t_1,t_2)$,[21] the expression for current can be written as

$$I_\alpha(t) = \frac{e}{\hbar}\int_{-\infty}^t dt_1 \text{Tr}[\Sigma_\alpha^<(t,t_1)G^>(t_1,t)$$
$$- \Sigma_\alpha^>(t,t_1)G^<(t_1,t) + \text{c.c.}] , \quad (9)$$

where

$$\Sigma_{\alpha,x,x'}^\gamma(t_1,t_2) = \sum_{i\alpha} V_{i\alpha,x}^*(t_1)V_{i\alpha,x'}(t_2)G_{i\alpha,i\alpha}^{0\gamma}(t_1,t_2) , \quad (10)$$

is the self-energy due to contact α and $\gamma \in r$ and $a, >, <$. Equation (9) has the meaning that the current in contact α is the electron in-scattering function due to contact α ($\Sigma_\alpha^<$) times the hole correlation function in the device ($G^>$) minus the hole in-scattering function due to contact α ($\Sigma_\alpha^>$) times the electron correlation function in the device ($G^<$).[22] A similar equation for the time-dependent current was obtained in Refs. 8 and 12 [Eq. (5.1) of Ref. 8 and Eq. (1) of Ref. 12]. Tr denotes trace over the spaptial coordinates, for example,

$$\text{Tr}[\Sigma_\alpha^<(t,t_1)G^>(t_1,t)]$$
$$= \sum_{x,x'\in \text{device}} \Sigma_{\alpha x,x'}^<(t,t_1)G_{x',x}^>(t_1,t) .$$

One could of course transform from the position representation to other representations such as the eigenstate representation. In general, we will not use any representation explicitly and simply treat the quantities Σ and G as matrices in some suitable representation. Equation (9) can be viewed as a generalized rate equation that allows us to handle nonlocal (in space and time) injection processes. Indeed if the functions $\Sigma_\alpha^<$ and $\Sigma_\alpha^>$ are both diagonal and local $[\Sigma_{min}^{>,<}(t_1,t_2)\sim \sigma_{min}^{>,<}(t_1)\delta_{mn}\delta(t_1 - t_2)]$, then Eq. (9) reduces to a simple rate equation

$$I_\alpha(t) = \frac{e}{\hbar}\sum_m \sigma_{\alpha,mm}^<(t)G_{mm}^>(t) - \sigma_{\alpha,mm}^>(t)G_{mm}^<(t) .$$

Note that the diagonal elements of $G^<$ and $G^>$ are proportional to the electron density and the hole density, respectively. In discussing the response to a sinusoidal driving signal, we find it convenient to transform the two-time coordinates to energy[17] and rewrite Eq. (9) in the form

$$I_\alpha(\omega) = \frac{e}{\hbar}\int_{-\infty}^{+\infty}\frac{dE}{2\pi}\int_{-\infty}^{+\infty}\frac{dE_1}{2\pi}\text{Tr}[G^r(E+\hbar\omega,E_1)\Sigma_\alpha^<(E_1,E) + G^<(E+\hbar\omega,E_1)\Sigma_\alpha^a(E_1,E)$$
$$- \Sigma_\alpha^<(E+\hbar\omega,E_1)G^a(E_1,E) - \Sigma_\alpha^r(E+\hbar\omega,E_1)G^<(E_1,E)] . \quad (11)$$

The advanced and retarded Green's and self-energy functions appearing in Eq. (6) are defined in the usual manner.[23] The equation is valid in general, i.e., in the presence of strong electron-electron interaction and strong electron-phonon interaction. The transformation from the time coordinates to energy coordinates follows the usual prescription,

$$F(E_1,E_2) = \int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{+\infty} dt_2 F(t_1,t_2)\exp[-i(E_1 t_1 - E_2 t_2)] .$$

For simplicity, we use the same symbols to denote the transformed functions.

B. Green's functions

To calculate the current, Eq. (11) has to be coupled with equations for the Green's functions G^r and $G^{>,<}$:[17]

$$E_1 G^r(r_1,r_2;E_1,E_2) - \int \frac{d\epsilon}{2\pi} H(r_1,\epsilon) G^r(r_1,r_2;E_1-\epsilon,E_2) - \int dr_3 \frac{dE_3}{2\pi} \Sigma^r(r_1,r_3;E_1,E_3) G^r(r_3,r_2;E_3,E_2)$$

$$= \delta(r_1-r_2)\delta(E_1-E_2) , \quad (12)$$

$$G^<(E_1,E_2) = \int_{-\infty}^{+\infty} \frac{dE_3}{2\pi} \int_{-\infty}^{+\infty} \frac{dE_4}{2\pi} G^r(E_1,E_3)\Sigma^<(E_3,E_4)G^r(E_4,E_2) , \quad (13)$$

where H is the Hamiltonian describing the conductor. The self-energy components appearing in Eqs. (12) and (13) are obtained by summing the components arising from the contacts [which appear in Eq. (11)] together with the components arising from electron-electron or electron-phonon interactions:

$$\Sigma^{>,<,r}(E_1,E_2) = \sum_\alpha \Sigma_\alpha^{>,<,r}(E_1,E_2) + \Sigma_\phi^{>,<,r}(E_1,E_2) . \quad (14)$$

Before we proceed we note that while Eq. (11) is applicable in general, Eqs. (12)–(14) can be used only when the system can be described by perturbation theory. For strongly interacting systems (e.g., Coulomb blockaded devices), the Green's functions have to be evaluated using nonperturbative techniques.[20]

C. Self-energy functions

One advantage of the energy representation is that it allows us to write down the in-scattering terms from the contacts in a simple form. Under steady-state conditions, these functions are purely diagonal in energy and Eq. (10) gives

$$-i\Sigma_\alpha^<(E,E') = \Gamma_\alpha(E)f_\alpha(E)\delta(E-E') ,$$
$$+i\Sigma_\alpha^>(E,E') = \Gamma_\alpha(E)[1-f_\alpha(E)]\delta(E-E') ,$$
$$\Sigma_\alpha^r(E,E') = -\tfrac{1}{2}[\Gamma_\alpha'(E)+i\Gamma_\alpha(E)]\delta(E-E') , \quad (15)$$
$$\Gamma_{\alpha,x,x'}(E) = 2\pi \sum_{i,\alpha} V_{i\alpha,x}^* V_{i\alpha,x'} \rho_{i\alpha}^0(E) ,$$

where the matrix $\Gamma_\alpha(E)$ describes the coupling of contact α to the conductor, while $\Gamma_\alpha'(E)$ is the Hilbert transform of $\Gamma_\alpha(E)$. $\rho_{i\alpha}^0(E) = -(1/\pi)G_{i\alpha,i\alpha}^{0r}(E)$ is the density of states at site i of contact α. The presence of a sinusoidal voltage of frequency ω in contact α introduces a correlation between energies[24] E and $E+n\hbar\omega$ so that the in-scattering function due to contact α, $\Sigma_\alpha^<(E+n\hbar\omega,E)$, develops off-diagonal components in energy. Physically one can see that the ac in-scattering function from contact α, $\Sigma_\alpha^<(E+n\hbar\omega,E)$, arises because electrons at energy $E-m\omega$, with a Fermi function $f_\alpha(E-m\omega)$, develops a sideband at energy E with a weighting factor $J_m(ev_{ac}/\hbar\omega)$ and a subband at energy $E+n\hbar\omega$ with a weighting factor $J_{n+m}(ev_{ac}/\hbar\omega)$. Then, neglecting the time dependence in the coupling between contact α and the device,

$$-i\Sigma_\alpha^<(E+n\hbar\omega,E)$$
$$= \sum_m J_{n+m}\left[\frac{ev_{ac}}{\hbar\omega}\right] J_m\left[\frac{ev_{ac}}{\hbar\omega}\right]$$
$$\times \Gamma_\alpha(E-m\hbar\omega)f_\alpha(E-m\hbar\omega) , \quad (16)$$

$$+i\Sigma_\alpha^>(E+n\hbar\omega,E)$$
$$= \sum_m J_{n+m}\left[\frac{ev_{ac}}{\hbar\omega}\right] J_m\left[\frac{ev_{ac}}{\hbar\omega}\right]$$
$$\times \Gamma_\alpha(E-m\hbar\omega)[1-f_\alpha(E-m\hbar\omega)] , \quad (17)$$

$$\Sigma_\alpha^r(E+n\hbar\omega,E)$$
$$= \sum_m J_{n+m}\left[\frac{ev_{ac}}{\hbar\omega}\right] J_m\left[\frac{ev_{ac}}{\hbar\omega}\right]\left[-\frac{1}{2}\right]$$
$$\times [\Gamma_\alpha'(E-m\hbar\omega)+i\Gamma_\alpha(E-m\hbar\omega)] , \quad (18)$$

where $\Gamma_\alpha(E)$ and $\Gamma_\alpha'(E)$ are defined in Eq. (15). The expressions for the self-energy components due to phase-breaking interactions depend on the nature of the interactions and the approximations used. For electron-phonon interactions in the self-consistent born approximation,[25]

$$\Sigma_\phi^{>,<}(r_1,r_2;E,E')$$
$$= \int \frac{d(\hbar\Omega_p)}{2\pi} D^{>,<}(\hbar\Omega_p) G^{>,<}(E-\hbar\Omega_p,E'-\hbar\Omega_p) . \quad (19)$$

The function $D^{>,<}$ is the Green's function for the phonon bath, which is assumed to be in equilibrium. If the phonon eigenstates are simple plane waves, we can write

$$D(r_1,r_2;\hbar\Omega_p)$$
$$= \sum_q |U_q|^2 [e^{-iq(r_1-r_2)} N_q \delta(\hbar\Omega_p - \hbar\Omega_q)$$
$$+ e^{+iq(r_1-r_2)}(N_q+1)\delta(\hbar\Omega_p+\hbar\Omega_q)] , \quad (20)$$

where N_q is the number of phonons with wave vector q and frequency ω_q and U_q is the potential "felt" by an electron due to a single phonon with wave vector q.

Equations (11)–(18) can be used to calculate the response of mesoscopic systems for arbitrary ac excitations. However, Eqs. (12)–(14) can be used only when the system can be described by perturbation theory and Eq. (19) is an expression for self-energy in the self-consistent Born approximation.[25] We will now specialize to the small-signal response and assume that $v_{\rm ac}$ is small.

III. SMALL-SIGNAL RESPONSE

A. Current expression

In this section we assume relatively featureless contacts, that is,

$$\Sigma_\alpha^r(E) = \Sigma_\alpha^r(E+\hbar\omega) = -i\Gamma_\alpha/2 \ . \tag{21}$$

This is often referred to as the wideband limit.[21] For small ac voltages, we can linearize Eq. (11) about the steady state to write

$$i_\alpha(\omega) = \frac{e}{\hbar}\int_{-\infty}^{+\infty}\frac{dE}{2\pi}\mathrm{Tr}[i_\alpha^{(1)}(E,\omega)+i_\alpha^{(2)}(E,\omega) \\ +i_\alpha^{(3)}(E,\omega)] \ , \tag{22}$$

where

$$i_\alpha^{(1)}(E,\omega) = \sigma_\alpha^<(E+\hbar\omega,E)[G^r(E+\hbar\omega)-G^a(E)] \ ,$$

$$i_\alpha^{(2)}(E,\omega) = i\Gamma_\alpha g^<(E+\hbar\omega,E) \ ,$$

$$i_\alpha^{(3)}(E,\omega) = g^r(E+\hbar\omega,E)\Sigma_\alpha^<(E) \\ -g^a(E+\hbar\omega,E)\Sigma_\alpha^<(E+\hbar\omega) \ .$$

We have used g and σ to denote the small-signal components of G and Σ, respectively. From here on we will use G and Σ to denote the steady-state quantities and not the total time-varying function as we have been doing so far. Since these are nonzero only if $E=E'$, we will write G and Σ with only one energy argument.

We have grouped the terms in Eq. (22) into three categories because each group has a different physical significance. The effect of oscillating a contact at frequency ω results in the following. Every energy E in the contact is now associated with sidebands at energies $E+n\hbar\omega$, where n is an integer. Correlated injection into the device due to electrons at energies E and $E+n\hbar\omega$ should be taken into account (first term). (ii) The electron density in the device changes with time. This causes correlated injection (at energies E and $E+n\hbar\omega$) from the device to the contact (second term). Note that the ac charge density in the device is given by $Q(\omega)=-ie\int dE\,\mathrm{Tr}[g^<(E+\hbar\omega,E)]$. (iii) As a result of the changing potential in the device region, the density of states in the device is affected and the third term represents injection from the contact at one energy to a changing density of states in the device.

B. Green's functions

Linearizing Eqs. (12) and (13) we obtain

$$g^r(E+\hbar\omega,E) = G^r(E+\hbar\omega)\sigma^r(E+\hbar\omega,E)G^a(E) \ , \tag{23}$$

$$g^<(E+\hbar\omega,E) = G^r(E+\hbar\omega)\sigma^<(E+\hbar\omega,E)G^a(E) \\ +g^r(E+\hbar\omega,E)\Sigma^<(E)G^a(E) \\ +G^r(E+\hbar\omega)\Sigma^<(E+\hbar\omega)g^a(E+\hbar\omega,E) \ . \tag{24}$$

C. Self-energy functions

For small ac voltages Eq. (17) reduces to

$$-i\sigma_\alpha^<(E+\hbar\omega,E) = \Gamma_\alpha\frac{f(E)-f(E+\hbar\omega)}{\hbar\omega}\frac{ev_{\rm ac}}{2} \\ = -i\sigma_\alpha^>(E+\hbar\omega,E) \tag{25}$$

for $n=1$, while the $n\neq1$ components can be neglected. Equation (19) can be written as

$$\sigma_\phi^{>,<}(r_1,r_2;E,E') = \int\frac{d(\hbar\Omega_p)}{2\pi}D^{>,<}(\hbar\Omega_p) \\ \times g^{>,<}(E-\hbar\Omega_p,E'-\hbar\Omega_p) \ . \tag{26}$$

Equations (22)–(26) can be used to describe the small-signal ac response including phase-breaking processes. While Eqs. (22) and (25) are applicable in general in the wideband limit of the contacts, Eqs. (23) and (24) can be used only when the system can be described by perturbation theory. Equation (26) is valid only in the self-consistent Born approximation.[25]

IV. CONNECTION TO SCATTERING THEORY

To make connection to the scattering theory result [Eq. (1) of this paper],[9] we assume a phase-coherent device with no ac potential inside the conductor, as discussed in Ref. 9, and apply the small-signal ac voltage to contact 1. Then (a) $g^r=0$ and the last term of Eq. (22) is identically zero and (b) $\sigma^<(k,E+\omega,E)$ has contributions only due to in scattering [Eq. (26)] from contact 1. Equation (24) then reduces to $g^<(E+\omega,E) = G^r(E+\omega)\sigma_1^<(k,E+\omega,E)G^a(E)$. Using these equations in Eq. (22), the small signal ac current is given by

$$i_\alpha(\omega) = \frac{e^2}{2h}\int dE\,\mathrm{Tr}[i\{G^r(E+\hbar\omega)-G^a(E)\}\Gamma_\alpha\delta_{\alpha1} \\ -\Gamma_\alpha G^r(E+\hbar\omega)\Gamma_k G^a(E)] \\ \times v_{\rm ac}\frac{f(E)-f(E+\hbar\omega)}{\hbar\omega} \ . \tag{27}$$

The scattering matrix of the device is related to the Green's function in the device by the relationship $s(E)=-I+i\Gamma^{1/2}G^r(E)\Gamma^{1/2}$.[22] It then follows that

$$[I\delta_{\alpha1}-s_{\alpha1}^\dagger(E+\hbar\omega)s_{\alpha1}(E)] \\ = \mathrm{Tr}[i\{G^r(E+\hbar\omega)-G^a(E)\}\Gamma_\alpha\delta_{\alpha1} \\ -\Gamma_\alpha G^r(E-\hbar\omega)\Gamma_1 G^a(E)] \ . \tag{28}$$

Making use of Eq. (27), Eq. (28) reduces to the scattering theory result [Eq. (1)].

V. SIMPLE EXAMPLES

We now illustrate the above formulation using two simple examples, including the effect of phase breaking. (i) The first is a one-dimensional resonant-tunneling diode [Fig. 2(a)] described by just one point in space as discussed in the Introduction. Here we show that the conductance versus frequency at low temperatures $[k_B T < (\Gamma_1 + \Gamma_2)]$ is modified by phase breaking, but on increasing the temperature $[k_B T \gg (\Gamma_1 + \Gamma_2)]$, the conductance is unaffected by phase breaking as discussed in the Introduction. (ii) The second is a one-dimensional resonant-tunneling diode with two energy levels [Fig. 3(b)]; here the cutoff frequency is affected by phase breaking. We restrict the calculation to the high-temperature limit $[k_B T \gg (\Gamma_1 + \Gamma_2)]$. In these examples we will assume that there is no ac potential inside the conductor. The point interaction for the electron-phonon interaction Hamiltonian is used, $H_{e-p} = \sum_{m,n,q} U(q) d_m^\dagger d_n [b_q + b_q^\dagger]$, where m and n represent single-particle states of the device and q represents the phonon modes. $U(q)$ is the strength of the interaction.

A. Example 1

We consider a one-dimensional resonant-tunneling diode with a single resonant level [Fig. 2(a)]. The ac conductance of a resonant-tunneling structure has been calculated previously in Refs. 4, 5, 7, 10, 11, and 15 in the phase-coherent limit only. These references, when applied to the particular example under consideration, would give essentially the same answers as ours only in the phase-coherent limit. Here we calculate the ac conductance in both the presence and the absence of phase breaking. The Green's function for this system in dc is given by $G^r(E) = 1/[E - \epsilon - \Sigma^r(E) + i(\Gamma_1 + \Gamma_2)]$. We then use Eqs. (22)–(26) to calculate the linear-response current by retaining only the imaginary parts of the self-energy (Σ_ϕ^r and σ_ϕ^r) corrections due to phonons. The phonon Green's function $D(\Omega)$ is assumed to be relatively featureless and for the plots in Fig. 2 $D(\Omega) = 3(\Gamma_1 + \Gamma_2) = 0.12$ meV.

Figure 2(b) is a plot of the low-temperature ac conductance as a function of frequency. As the Fermi level has been taken to lie below the resonant energy, the ac conductance initially rises due to the increasing density of states above the chemical potential and then eventually decreases. When phase breaking is included, the peak conductance decreases, but the conductance increases at higher frequencies when compared to the phase-coherent case [Fig. 2(b)]. This can be understood by noting that in the presence of phase breaking, (i) the density of states decreases at resonance and increases away from the resonance, except at the Fermi energy at very low temperatures ($kT \ll \Gamma$), and (ii) the ac self-energy due to phonons, $\sigma_\phi^<(E + \omega, E)$, is small for large ω.

In the high-temperature limit, the in scattering due to phonons at a given energy is nearly equal to the out scattering at the same energy. Then, $\sigma^r = 0$ and from Eq. (23), $g^r \sim 0$. As a result, $i_\alpha^{(2)}(E, \omega) = 0$. From Eqs. (22),

$$i_2(\omega) = -\frac{2\Gamma_2}{\hbar} Q(\omega)$$

where

$$Q(\omega) = e \int_{-\infty}^{+\infty} \frac{dE}{2\pi} [-ig^<(E + \hbar\omega, E)] .$$

The factor of 2 in the expression for i_2 accounts for spin degeneracy. Also, we assume that the phonon function D is nearly constant in the energy range of interest; we can then write, from Eq. (26),

$$\sigma_\phi^<(E + \hbar\omega, E) = D \int_{-\infty}^{+\infty} dE [-ig^<(E + \hbar\omega, E)]$$
$$= \Gamma_\phi Q(\omega)/e \qquad (29)$$

since $2\pi D = \Gamma_\phi$.[26] Noting that the Green's function is given by $G^r(E) = 1/[(E - E_r) + i(\Gamma_1 + \Gamma_2 + \Gamma_\phi)/2]$ and using Eqs. (23), (24), and (29), we obtain

$$Q(\omega) = \frac{ev_{ac}}{2} f' \frac{\Gamma_1}{\Gamma_1 + \Gamma_2 + \Gamma_\phi - i\hbar\omega} + \frac{\Gamma_\phi Q(\omega)}{\Gamma_1 + \Gamma_2 + \Gamma_\phi - i\hbar\omega} ,$$
$$(30)$$

so that

$$i_2 = \frac{e^2}{\hbar} v_{ac} f' \frac{\Gamma_1 \Gamma_2}{\Gamma_1 + \Gamma_2 - i\hbar\omega} ,$$

which is exactly the same result obtained for coherent transport [see Eq. (3)], thus showing that phase-breaking processes do not have a significant effect on current in the high-temperature limit [Fig. 2(c)].

B. Example 2

We now consider a resonant-tunneling device with two resonant energy levels ϵ_a and ϵ_b [Fig. 2(b)] such that $\Gamma_{aa}, \Gamma_{bb} \ll kT \ll \epsilon_b - \epsilon_a$ so that $f(\epsilon_a) < 1$ and $f(\epsilon_b) \sim 0$. The coupling to the contacts is represented by $\Gamma_{a1}, \Gamma_{a2}, \Gamma_{b1}, \Gamma_{b2}$, and $\Gamma_{xx} = \Gamma_{1aa} + \Gamma_{2aa}$, where $x \in a, b$. The linear-response current vs frequency of such a structure is peaked around $\hbar\omega \sim 0$ and $\hbar\omega \sim \epsilon_b - \epsilon_a$ [Fig. 3(b)]. The high-frequency peak exists because an electron incident in contact 1 at energy ϵ_a has a sideband at energy ϵ_b and the transmission through the device is peaked at both these energies. On raising the Fermi energy, the low-frequency peak diminishes because occupancy of the lower level approaches unity and the electron density cannot change significantly [Fig. 3(b)]. As in the previous example, the low-frequency conductance peak is unchanged due to phonon scattering and here we will be concerned with the high-frequency conductance peak. The formalism in Refs. 4, 5, 7, 10, 11, and 13, which study phase-coherent transport, would have given the same results when applied to this problem only in the phase-coherent limit. Here we study the effect of phonon scattering on the high-frequency peak [Fig. 3(c)]. The dominant scattering mechanism is assumed to be due to phonons of energy $\sim \epsilon_b - \epsilon_a$. For $\omega \sim \epsilon_b - \epsilon_a$, from Eq. (26), the self-energy due to phonon scattering $\sigma_\phi^{>,<}(E + \hbar\omega, E) \sim 0$. This implies $\sigma_\phi^r(E + \hbar\omega, E) \sim 0$ and from Eq. (23), $g^r \sim 0$. It then follows from Eqs. (22) that

$$i_2(\omega) = -\frac{2\Gamma}{\hbar} Q_{ba}(\omega)$$

where

$$Q_{ba}(\omega) = e \int_{-\infty}^{+\infty} \frac{dE}{2\pi} [-ig_{ba}^<(E+\hbar\omega, E)] .$$

The factor of 2 in the expression for i_2 accounts for spin degeneracy. Noting that the Green's functions are given by $G_{xx}^r(E) = 1/[(E-E_x)+i(\Gamma_{1xx}+\Gamma_{2xx}+\Gamma_{\phi x})/2]$, where $x \in a, b$, and $\Gamma_{\phi a} = 0$ and $\Gamma_{\phi b} = D/2(1-f_a)$, where f_a is the Fermi function at energy ϵ_a, it follows from Eqs. (23), (24), and (29) that the current is given by

$$i_2(\omega) = -\frac{\Gamma_{2ab}}{\hbar} Q_{ba}(\omega) = \frac{e^2}{\hbar} \frac{v_{ac}}{\hbar\omega} f_a \frac{\Gamma_{1ba}\Gamma_{2ab}}{\frac{\Gamma_{1aa}+\Gamma_{1bb}+\Gamma_{2aa}+\Gamma_{2bb}+\Gamma_{\phi b}}{2} - i(\hbar\omega - \Delta)} , \qquad (31)$$

where $\Delta = \epsilon_b - \epsilon_a$. From this expression, it is clear that phonon scattering has two effects on the frequency response [Fig. 3(c)] of the high-frequency conductance peak: (i) the peak height reduces and (ii) the width of the frequency response now increases from $(\Gamma_{1aa}+\Gamma_{1bb}+\Gamma_{2aa}+\Gamma_{2bb})/2$ to $(\Gamma_{1aa}+\Gamma_{1bb}+\Gamma_{2aa}+\Gamma_{2bb}+\Gamma_{\phi b})/2$. The peak height decreases because the component of the electronic wave function at energy $\sim \epsilon_b$ can scatter down to energy $\sim \epsilon_a$, due to phonon scattering, thus reducing the magnitude of the correlation function Q_{ba}.[27] As a result of phonon scattering, the density of states $[(1/\pi)\text{Im}\{G^r\}]$ increases away from the resonance at energy ϵ_b. This causes the correlation function at nonresonant energies to increase.[27] As the Fermi energy increases, the leakage rate of the electron wave function from energy ϵ_b to ϵ_a becomes smaller and the high-frequency peak with phonon scattering approaches the phase-coherent value [compare Figs. 3(c) and 3(d)].

VI. CONCLUDING REMARKS

We have presented a general formulation based on the NEGF formalism that allows us to describe the ac response of mesoscopic systems including arbitrary amounts of phase-breaking and dissipative processes. In the case of a phase-coherent device, we show that our equation for current reduces to the linear-response result derived in Ref. 9. The formulation is illustrated by two simple examples: (i) a one-dimensional resonant-tunneling device with a single level, where the small-signal current is affected by phonon scattering at low temperatures, but is not affected in the high-temperature limit, and (ii) a resonant-tunneling device with two levels where the small-signal current is affected by phonon scattering.

ACKNOWLEDGMENT

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